PROJECT NUMBER: 1754
PROJECT TITLE: Spectroscopic Studies of Tobacco and Smoke Components
PROJECT LEADER: J. B. Wooten
WRITTEN BY: R. L. Bassfield
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SOLUTION NMR

A. **Objective**: Use NMR to determine the optical purity of extracted nicotine.

B. **Results**: The first of two samples submitted by R. Izac for optical purity analysis contained impurities which caused spectral broadening upon the addition of the chiral shift reagent. Therefore a purity measurement was not obtainable. The second sample, free of impurities, displayed good resolution over the course of the additions of shift reagent and no splitting of the N-methyl resonance was observed.

C. **Conclusions**: This would indicate that the second sample was one isomer or predominantly one isomer; since a small amount of one might be hidden in the base of the taller peak.

D. **Plans**: A novel approach to optical purity measurements of alkaloids, by NMR, was recently reported. This procedure is based on the inclusion of these compounds with β-cyclodextrin which causes differences in the chemical shifts of the two enantiomers. It is reported that little or no broadening occurs with resolution at several sites. If successful, we plan to use this procedure as a model for our nicotine determinations.

A. **Objective**: Determine the structure of an unknown glucoside isolated from bright tobacco.

B. **Results**: ^{1}H, ^{13}C and 2D NMR experiments have been employed to identify this compound as a sesquiterpene glucoside with the aglycone possibly derived from solavetivone. Comparison of our data with a literature reference was favorable. Preliminary 2D results indicate the site of the glucoside linkage is the carbon atom adjacent to the carbonyl in the cyclohexenone ring, and not on the sidechain as expected.

C. **Plans**: Additional experiments will be performed in order to confirm the site of the glucoside linkage.

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